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Title: A Turbulent Mix-Model for Re-stabilized Flows

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Gore, Robert Allen

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A Turbulent Mix-Model for Re-stabilized Flows

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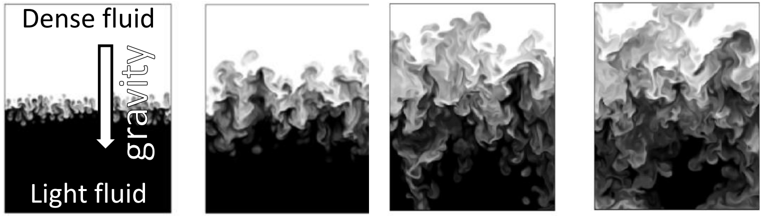
Rob Gore

19 May 2021

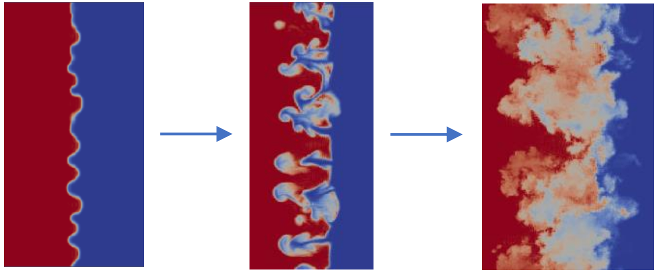
Turbulent Mixing

- Hydrodynamic instabilities are a common driver of material mixing
  - Acceleration Driven (Rayleigh-Taylor)

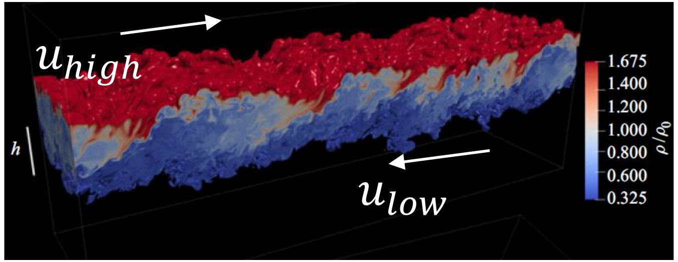


Source: Dalziel et al. (1999)

  - Shock-Driven (Richtmyer-Meshkov)



Shear-Driven (Kelvin-Helmholtz)



source: Baltzer and Livescu (2020)

- Directly computing hydrodynamics at the resolutions required to accurately capture turbulence mixing is typically impractical
  - Engineering Approach: Reynolds-Averaged Navier-Stokes (RANS)
  - Solve for ensemble-averaged solutions

BHR Modeling Approach

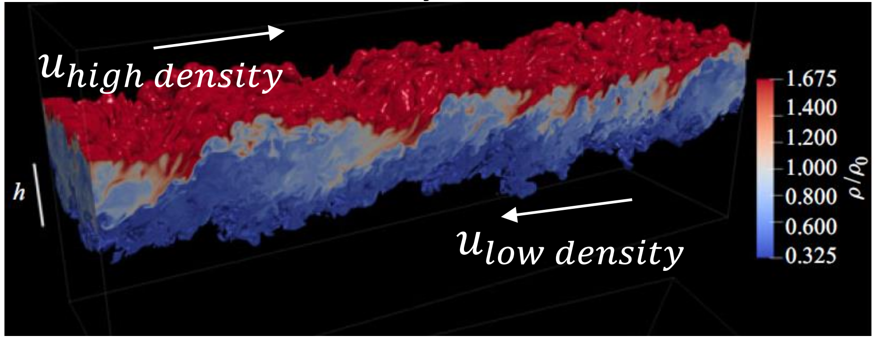
$$f_{,j} = \frac{\partial f}{\partial x_j}$$

- Reynold-Averaged Navier-Stokes
  - Navier-Stokes Momentum: $\frac{\partial \rho u_i}{\partial t} - \left(\rho u_j u_i - P\delta_{ij} - \tau_{ij}\right)_{,j} = 0$
  - Apply averaging and assume small viscosity:
    - $(\bar{\rho}\tilde{u}_i)_{,t} - \left(\bar{\rho}\tilde{u}_j\tilde{u}_i - \bar{P}\delta_{ij} - \bar{\rho}\tilde{R}_{ij}\right)_{,j} = 0$
    - $\bar{f}$: ensemble average of f, $\tilde{f} = \overline{\rho f}/\bar{\rho}$
    - f' and f'' are fluctuations about the mean $f = \tilde{f} + f'' = \bar{f} + f'$
  - Reynolds Stress: $\tilde{R}_{ij} = \overline{\rho u_i'' u_j''}/\bar{\rho}$
    - Measure of velocity fluctuations in the flow
    - Turbulent kinetic energy: $K = \tilde{R}_{ii}/2$
    - Unknown; must be modeled
      - $\frac{\partial(\bar{\rho}\tilde{R}_{ij})}{\partial t} + \left(\bar{\rho}\tilde{u}_j\tilde{R}_{ij}\right)_{,j} = \cdots$

BHR Modeling Approach

- BHR is an empirical model
  - $\frac{\partial(\bar{\rho}\tilde{R}_{ij})}{\partial t} + \left(\bar{\rho}\tilde{u}_j\tilde{R}_{ij}\right)_{,j} = -\frac{\partial}{\partial x_k}\left(\overline{\rho u_i'' u_j'' u_k''}\right) + \ldots$
  - Unknown terms, e.g. $\overline{\rho u_i'' u_j'' u_k''}$

DNS of a turbulent shear layer



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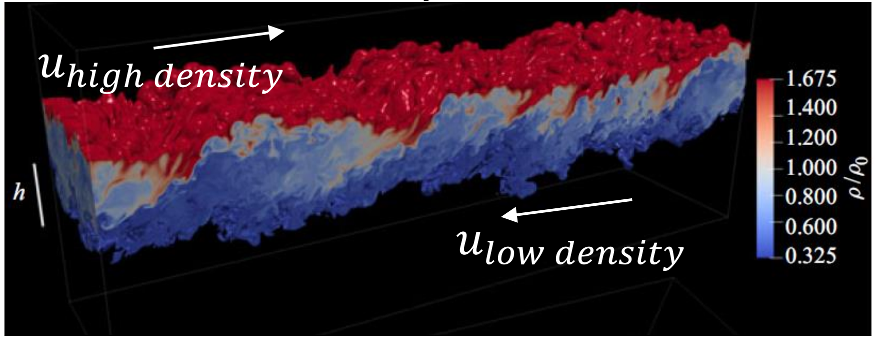
  - Unknown terms, e.g. $\overline{\rho u_i'' u_j'' u_k''}$
  - Make an ansatz (*gradient diffusion hypothesis*) that turbulent velocity fluctuations tend to transport quantities along scalar gradients,
    - $\overline{\rho u_i'' u_j'' u_k''} \approx -C_\mu \bar{\rho} \nu_t \frac{\partial \tilde{R}_{ij}}{\partial x_k}$
    - ν_t : turbulent viscosity (turbulent length scale × turbulent velocity scale)
  - Then tune coefficient C_μ such that BHR matches relevant DNS and experiments
    - Assumes C_μ a universal constant – not reliable in transitional flows

DNS of a turbulent shear layer



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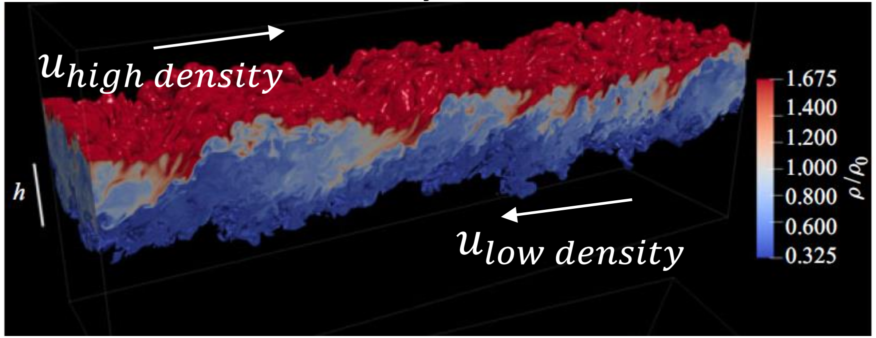
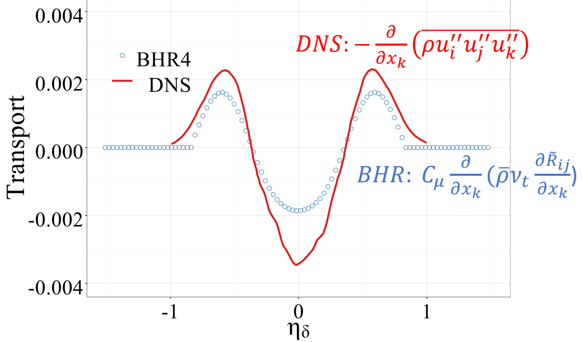
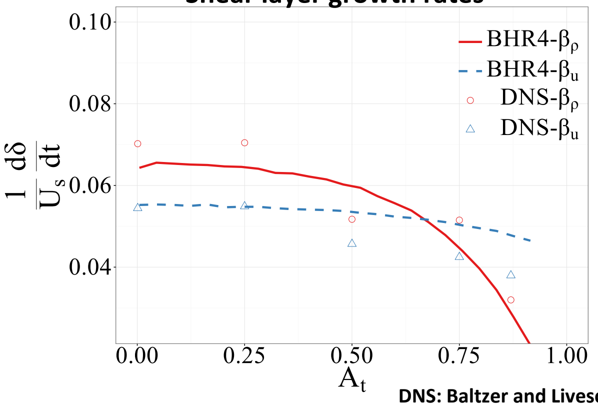


source: Baltzer and Livescu (2020)

Transport term across a uniform density shear layer



Shear layer growth rates



DNS: Baltzer and Livescu (2020)

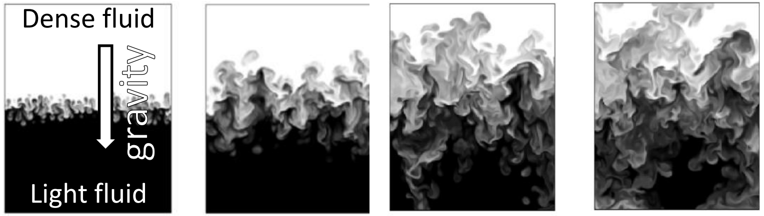
Variables Evolved in BHR

- BHR3.1
  - Tracks closure models for a number of turbulent variables
    - $\tilde{R}_{ij}$: Reynolds stress – amplitude of velocity fluctuations in the flow $\quad \tilde{R}_{ij} = \frac{\overline{\rho u_i'' u_j''}}{\bar{\rho}}$; $\left(\frac{cm^2}{s^2}\right)$
      - Momentum transport by turbulence
    - a_i : turbulent mass flux – mass transport due to velocity fluctuations $\quad a_i = \frac{\overline{\rho' u_i'}}{\bar{\rho}}$; $\left(\frac{cm}{s}\right)$
      - Mass transport by turbulence
    - S_T; S_D : Transport and dissipation lengthscales in the turbulence $\quad S_D = \frac{K^{\frac{3}{2}}}{\varepsilon}$; (cm)
    - b : density-specific volume covariance $\quad b = -\overline{\rho' v'}$; $(-)$
      - Measure of density fluctuations

- BHR4
  - Adds species-specific quantities:
    - a_i^k : turbulent flux of material mass for material k $\quad a_i^k = -\frac{\overline{\rho u_i'' c^{k''}}}{\bar{\rho}}$; $\left(\frac{cm}{s}\right)$
    - b^k : correlation between density and mass fraction fluctuations for material k $\quad b^k = -\frac{\overline{\rho' c^{k'}}}{\bar{\rho}}$; $(-)$

Turbulent Mass Flux, a_i

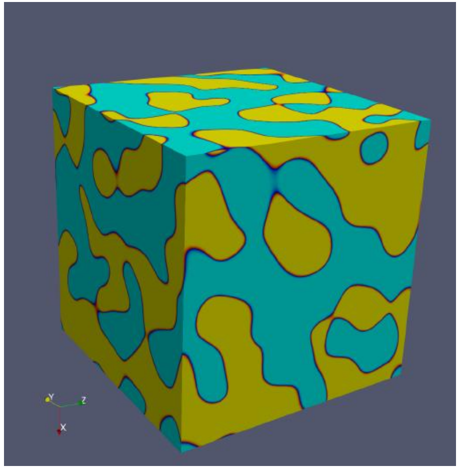
- The turbulent mass flux is a measure of material advection by turbulence
- In incompressible Rayleigh-Taylor flows there is negligible average velocity, $\bar{u} \approx 0$
  - Volume falling dense fluid equals volume of rising light fluid
  - The continuity equation becomes,
    - $\frac{\partial \bar{\rho}}{\partial t} + \left(\bar{\rho} a_j\right)_{,j} = 0$
    - The turbulent mass flux a_i is effectively the advection velocity of mass in the frame where there is no background bulk advection velocity.
  - Advection velocity of $\bar{\rho}$: $\tilde{u}_i \;=\; \underbrace{\bar{u}}_{\text{Volume averaged velocity}} \;+\; \underbrace{a_i}_{\text{Additional material movement due to mix}}$
    - Generally : $\frac{\partial \bar{\rho}}{\partial t} + \left(\bar{\rho} \tilde{u}_j\right)_{,j} = 0$



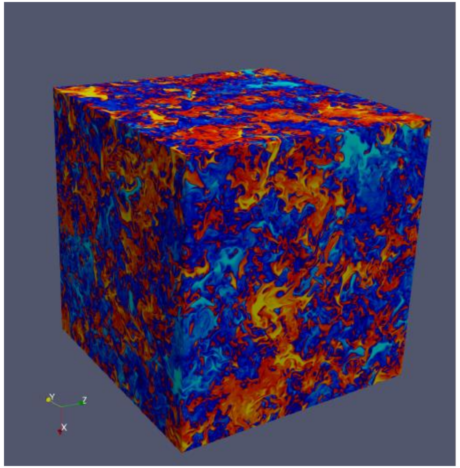
Source: Dalziel et al. (1999)

b as a mix-metric

- $b = -\overline{\rho' v'}$ is often employed as a measure of molecular mix
  - b is a measure of density variations; $b \approx \frac{\overline{\rho'\rho'}}{\bar{\rho}^2}$ in flows with $\frac{|\rho'|}{\bar{\rho}} \ll 1$
  - The more molecularly mixed a flow is, the lower the density fluctuations are
    - Lower b tends to correspond to a more molecularly mixed state



High b: Materials are intermingled but not mixed



[1]

Low b: Materials are well mixed

[1] Kurien et al. 2019 'Local Wavenumber Turbulence Model Implementation in xRAGE: L3 Milestone Report'

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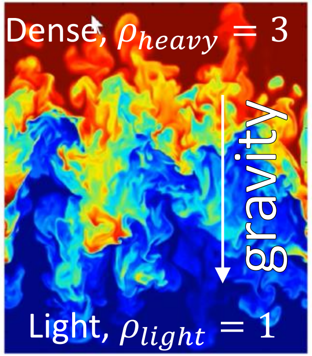
  - b is a measure of density variations; $b \approx \frac{\overline{\rho'\rho'}}{\bar{\rho}^2}$ in flows with $\frac{|\rho'|}{\bar{\rho}} \ll 1$
  - The more molecularly mixed a flow is, the lower the density fluctuations are and the lower b is

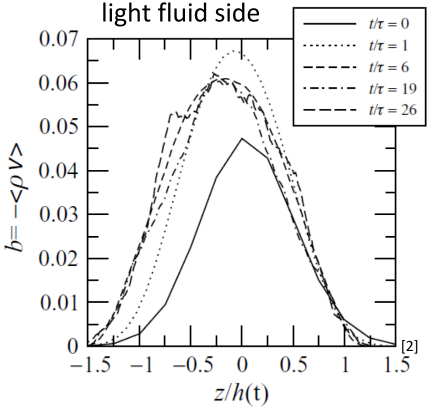
- b is a hydrodynamic quantity and there are some limitations to using b to infer material mixing

$A_t = 0.5$ Rayleigh-Taylor mixing layer



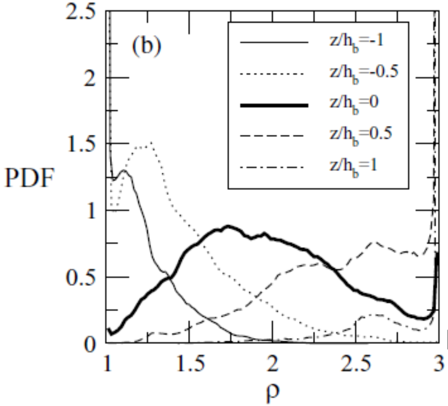
Source: Livescu (2011)

Profile of b across the mixing layer
- b is maximum near the center of the mixing layer, biased towards light fluid side



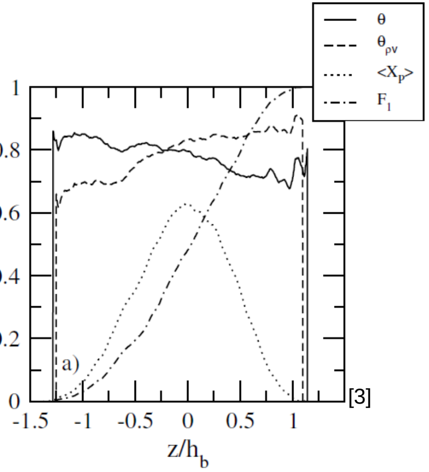
[2]

PDF of density at different heights
- Peaks closer to $\rho = 2$ correspond to a more mixed state
- Centerline is most mixed
- Light fluid side mixes more than heavy fluid side



[3]

Measuring mix from b can require additional modeling
- $\theta_{\rho v} = 1 - \frac{b}{b_{nomix}}$ (dashed line)
- Ristorcelli's PDF methods



[3]

[1] Kurien et al. 2019 'Local Wavenumber Turbulence Model Implementation in xRAGE: L3 Milestone Report'
[2] Livescu et al. 2009 'High-Reynolds number Rayleigh–Taylor turbulence'
[3] Livescu and Petersen 2010 'New phenomena in variable-density Rayleigh–Taylor turbulence'

Variables Evolved in BHR

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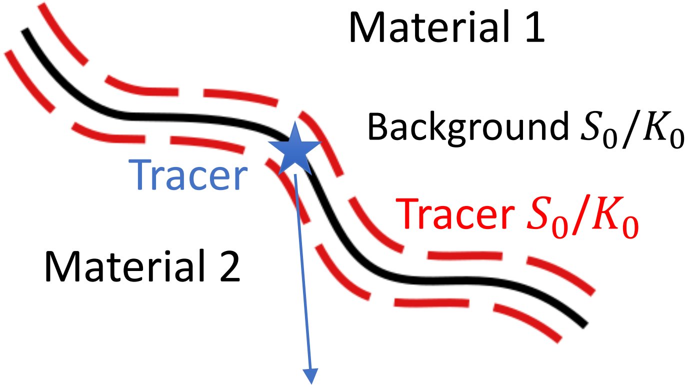
    - a_i : turbulent mass flux – mass transport due to velocity fluctuations $\quad a_i = \frac{\overline{\rho' u_i'}}{\bar{\rho}}\ ;\ \left(\frac{cm}{s}\right)$
    - $S_T; S_D$: Transport and dissipation lengthscales in the turbulence $\quad S_D = \frac{K^{\frac{3}{2}}}{\varepsilon}\ ;\ (cm)$
    - b : density-specific volume covariance $\quad b = -\overline{\rho' v'}\ ;\ (-)$

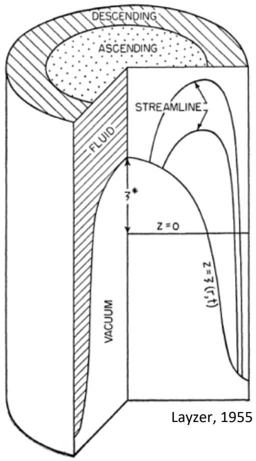
Need initial conditions for these ($S_0; K_0 = \frac{\tilde{R}_{nn}}{2}$)

- BHR4
  - Adds species-specific quantities:
    - a_i^k : turbulent flux of material mass for material k $\quad a_i^k = -\frac{\overline{\rho u_i'' c^{k''}}}{\bar{\rho}};\ \left(\frac{cm}{s}\right)$
    - b^k : correlation between density and mass fraction fluctuations for material k $\quad b^k = -\frac{\overline{\rho' c^{k'}}}{\bar{\rho}}\ ;\ (-)$

Initial Conditions

- Need initial lengthscale (S_0) and initial turbulent kinetic energy (K_0)
  - Often S_0 and K_0 are tuned to match experiments
- Goncharov (modal model 1)
  - Potential flow model for parabolic bubbles on the interface
  - A Lagrangian tracer particle is placed on the material interface, and a laminar model for the interface evolution is tracked at the tracer
  - Once the Reynolds number of the interface growth is large enough, turns on BHR and sets S and K within a small zone about the interface
    - The normal S_0/K_0 prescription is used for the background values, so should set these to be fairly small
  - Some limitations
    - Non-linear coupling between modes is neglected. May be best to approximate multimode perturbations by single mode
    - Limited to small amplitude to wavelength ratios
- Z-model (modal model 2) – vortex-sheet model
  - Allows large amplitudes and multimode interactions
  - Stability can be an issue
- Tracer-BHR – Approximate solution to BHR used with modal model
  - Delays turning on BHR until the interface has grown large enough to resolve on the grid.



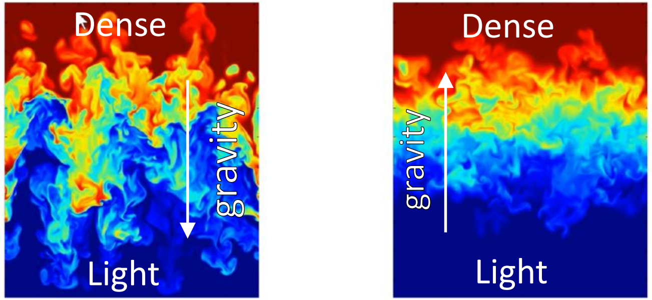


Layzer, 1955

Changes in BHR4 - Modeling material transport

- BHR3.1
  - Transport of averaged material mass-fraction $\tilde{c}^k$ modeled by gradient-diffusion:
    - $$\underbrace{\frac{\partial(\bar{\rho}\tilde{c}^k)}{\partial t} + \left(\bar{\rho}\tilde{u}_j\tilde{c}^k\right)_{,j}}_{\text{Advection of material}} = \underbrace{-\left(\overline{\rho u_j'' c^{k''}}\right)_j \approx C_\mu\left(\bar{\rho}S_T\sqrt{K}\tilde{c}^k_{,j}\right)_{,j}}_{\text{Mixing of material}}$$
  - Material mixing does not always behave like diffusion

$A_t = 0.5$ Rayleigh Taylor instability with gravity reversal



Source: Livescu (2011)

BHR4 - Multispecies Material Transport

- Track new closure equations for species transport and fluctuations
  - Transport of averaged material mass-fraction $\tilde{c}^k$:
    - $\frac{\partial(\bar{\rho}\tilde{c}^k)}{\partial t} + \left(\bar{\rho}\tilde{u}_j\tilde{c}^k\right)_{,j} = \left(\bar{\rho}a_j^k\right)_{,j}$
    - $a_i^k = -\frac{\overline{\rho u_i'' c^{k''}}}{\bar{\rho}}$: turbulent flux of species mass fraction, for species k
    - $b^k = \overline{c^{k''}}$: turbulent fluctuation in species mass fraction, for species k
  - For constant species densities, ρ^k, the species terms are directly related to the turbulent mass flux, a, and turbulent density fluctuations, b
    - $a = \bar{\rho}\sum_k \frac{a^k}{\rho^k}$; $b = \bar{\rho}\sum_k \frac{b^k}{\rho^k}$
    - Given the exact unclosed equations for a^k and b^k (Cihonski et al. 2015), and assuming that BHR4.0 should be consistent with the a and b equations of BHR3.1 in incompressible flows, directly yields equations for a^k and b^k
  - xRage is a compressible code (ρ^k are not constant) so we still track a and b

Reversed Gravity Rayleigh-Taylor

- Dense fluid above light fluid
  - Initially gravity is downward, driving mixing
  - After some time, gravity reverses direction and stabilizes the mixing layer

- Initial conditions
  - All test cases shown here are initialized from the Goncharov model (modal model 1)
    - Potential flow model for laminar bubble evolution
  - At $Re_h = 20$, the Goncharov model initializes BHR with a TKE based on the bubble velocities and $S_T = S_D$ set equal to the bubble amplitude

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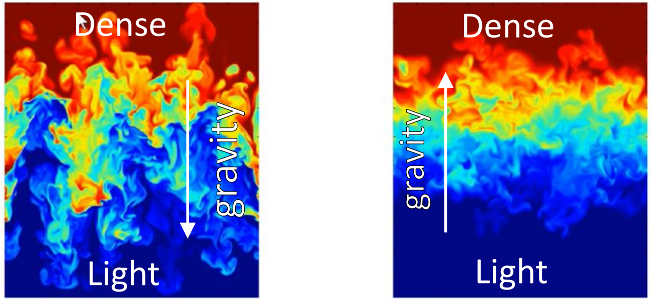

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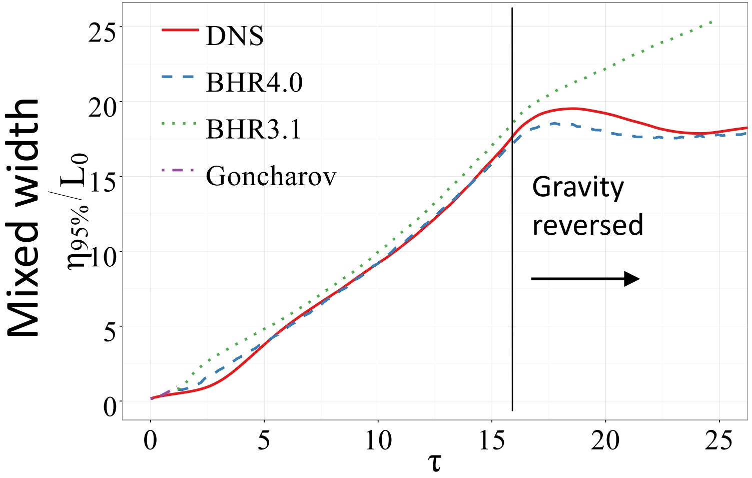
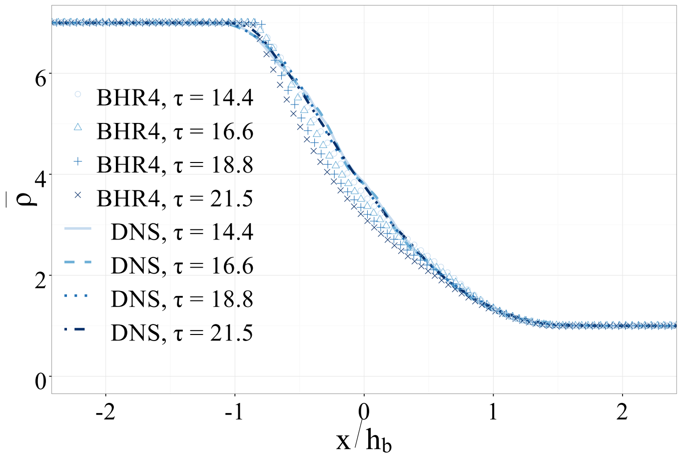
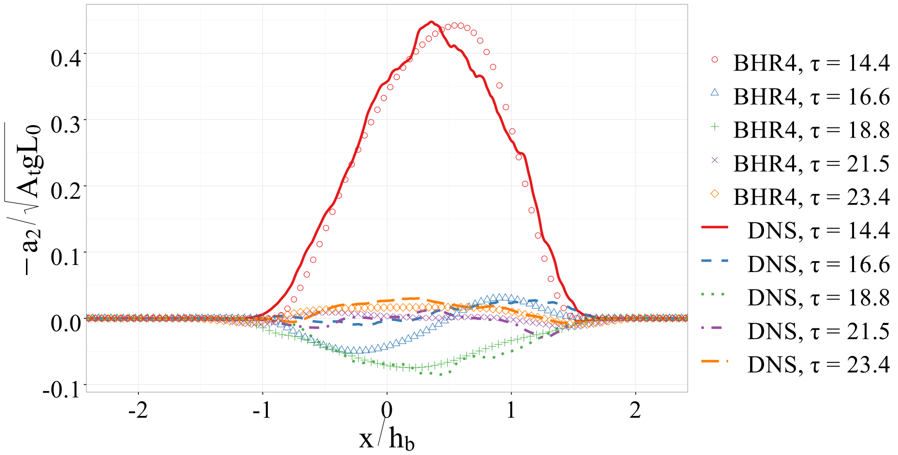


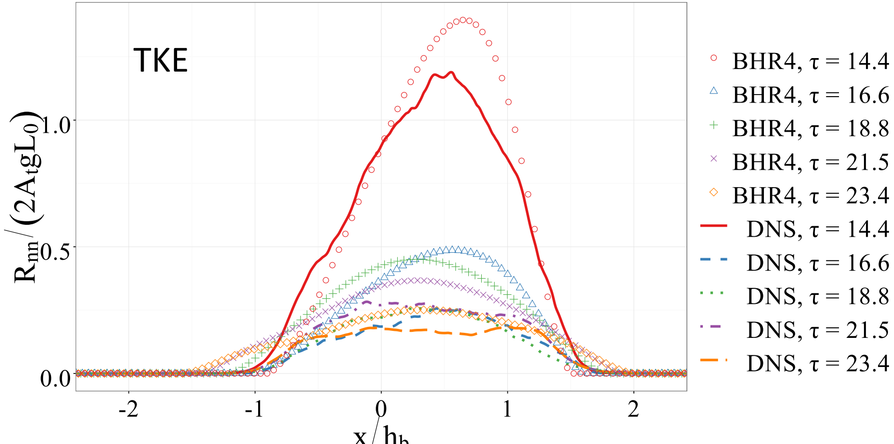
Statistical Profiles Post-Gravity Reversal (BHR4.0)

Density



Turbulent Mass Flux





Gravity reversed at $\tau = 14.4$

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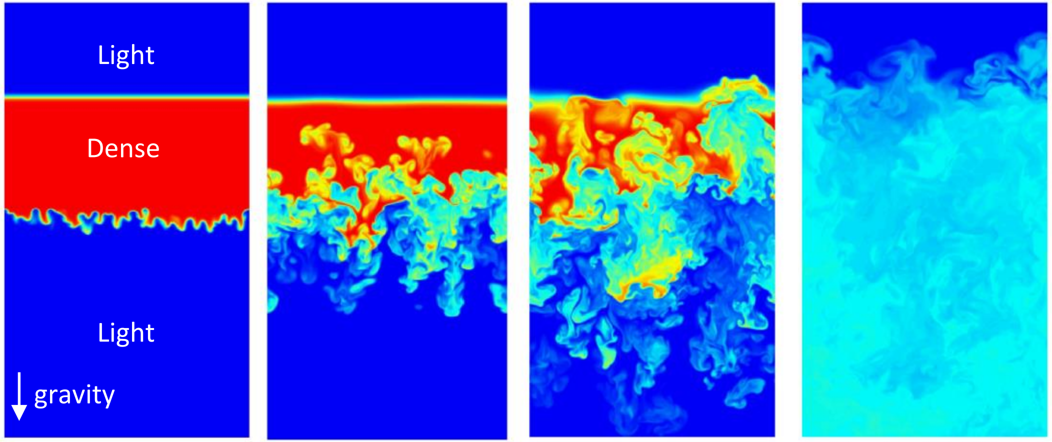
Shell Breakup Due to Gravity

- Dense fluid layer suspended in light fluid
  - Low half of the shell is unstable and begins mixing
  - Eventually the lower mixing layer impinges on the upper interface, driving mixing at the stable interface
  - Compared to DNS of Youngs (2017)
  - $\frac{\rho_{heavy}}{\rho_{light}} = 3$

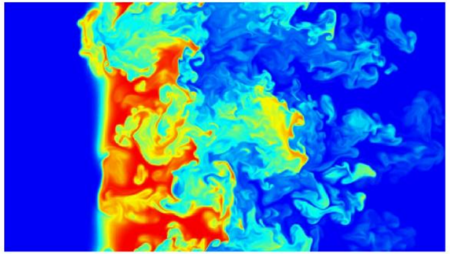


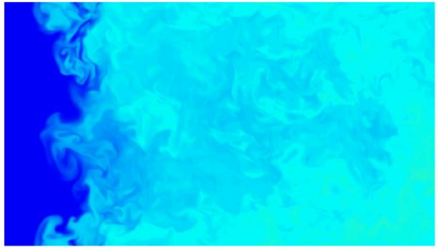
(a) τ=1 (b) τ=2.5 (c) τ=4 (d) τ=10

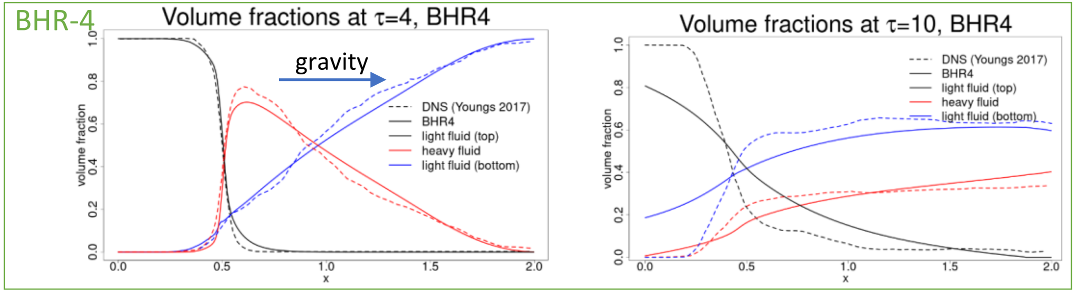
Source: Youngs (2017)

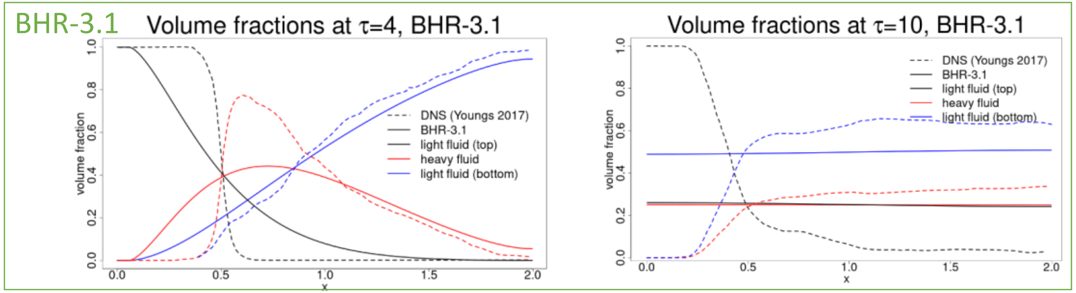
Shell Breakup Due to Gravity

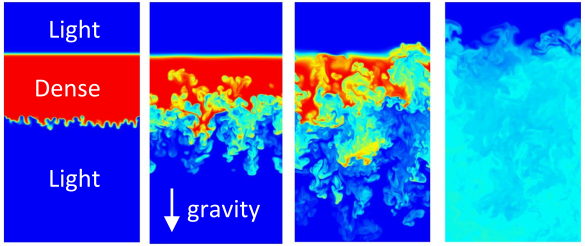
- Dense fluid layer suspended in light fluid
  - Compared to DNS of Youngs (2017)
  - Lower half of the shell is unstable and begins mixing, eventually impinging on the upper stable interface
  - The stability of the upper interface resists mixing and remains relatively sharp even after the unstable mixing layer reaches it.
  - At $\tau = 4$ (first column of images), BHR4 captures the sharp upper interface relatively well, whereas BHR3.1 generates too much mixing at the interface.
  - At $\tau = 10$ (second column of images), BHR4 retains the general structure of the DNS, whereas BHR3.1 has fully mixed to a uniform state.











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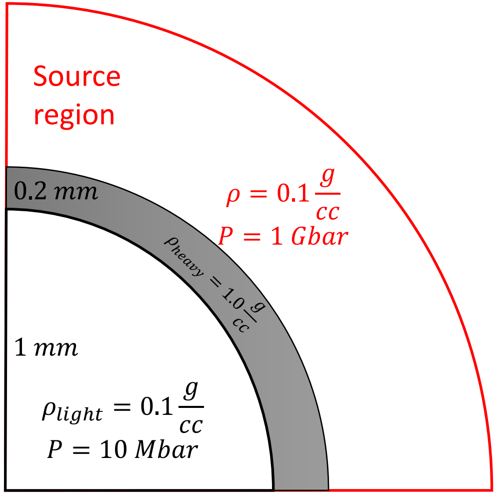
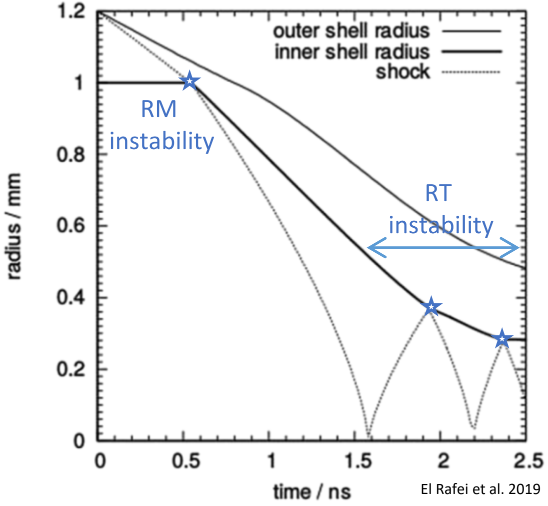
Source: Youngs (2017)

Spherical Implosion

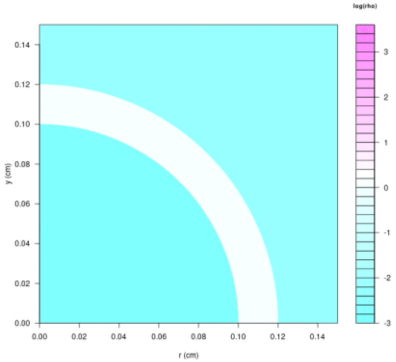
- Implosion of a dense spherical shell
  - Mix of RM (shock-driven) and RT (acceleration-driven) instabilities
  - Implosion driven by prescribed, time-varying source region
  - 1d spherical problem in RANS, compared to 3D LES (El Rafei et al. 2019)
  - Variations on this problem previously used as hydrodynamics validation test for xRage (Joggerst et al. 2014).

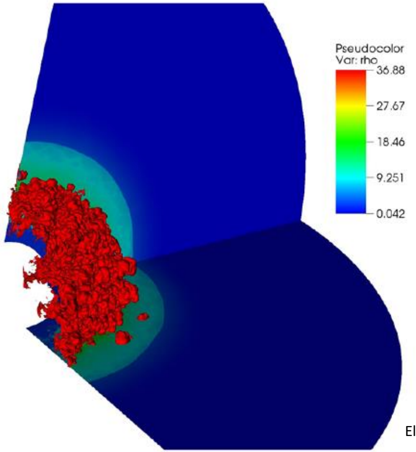


Interface and shock locations in 1D simulation with no mixing



El Rafei et al. 2019





El Rafei et al. 2019

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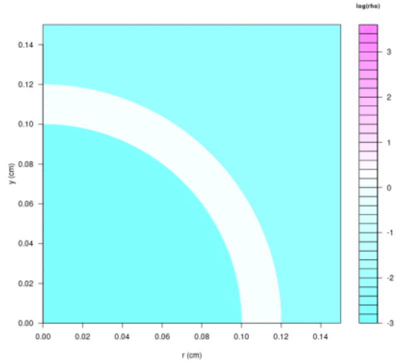
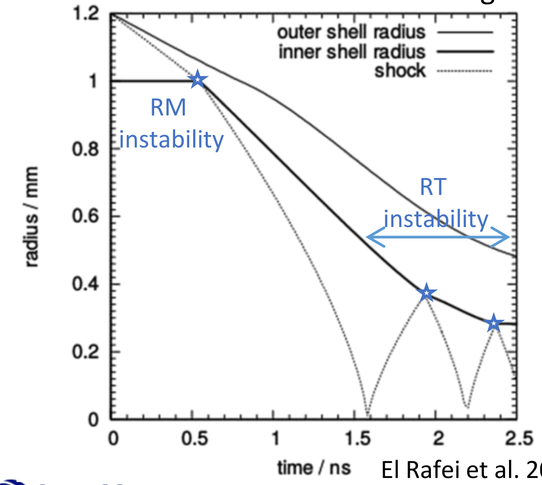
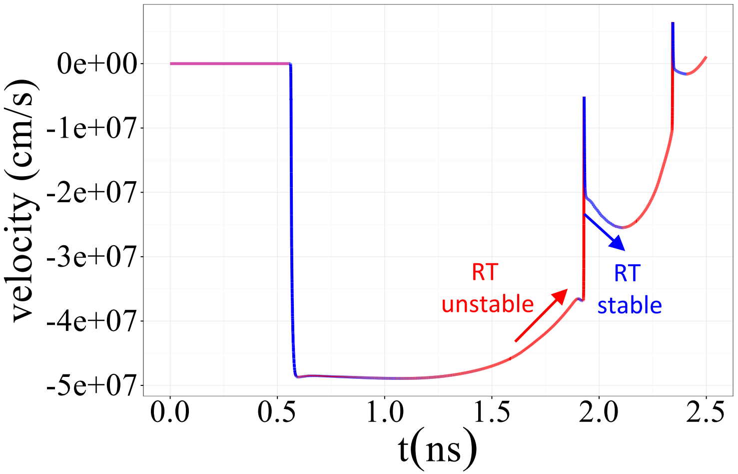


Interface and shock locations in 1D simulation with no mixing



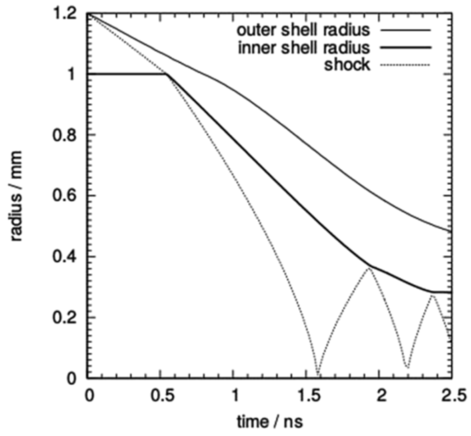
El Rafei et al. 2019

Interface velocity

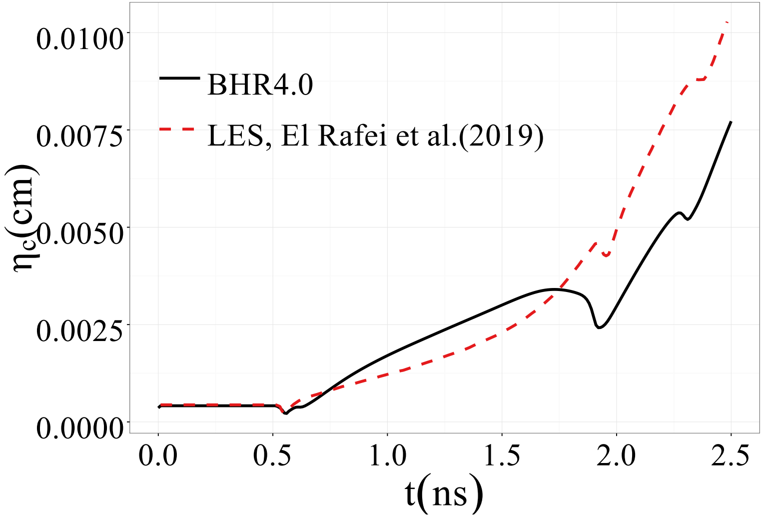


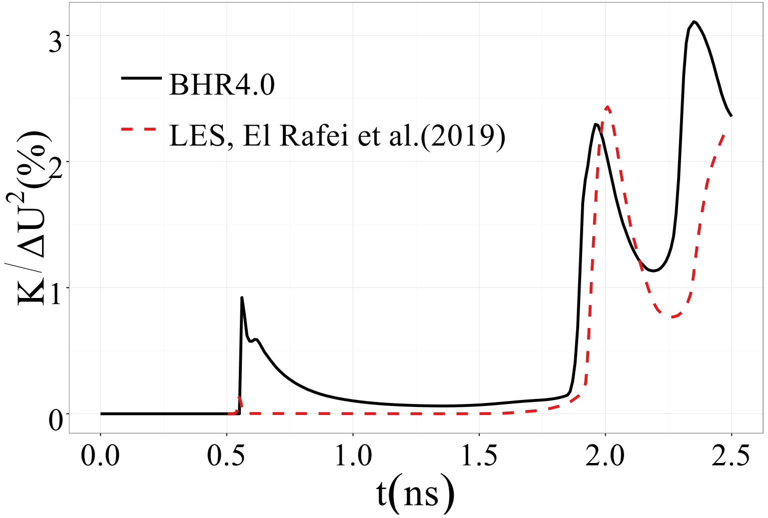
Spherical Implosion

- 1D RANS of implosion of a spherical shell
  - Comparing statistics of mixing layer at interior surface of shell to LES of (El Rafei et al. 2019)
  - Reasonable agreement with turbulent kinetic energy and mixing layer growth rates
  - The mixing layer shrinking at $t \approx 1.75 - 2.0ns$ results from a mixture of de-mixing, shock compression, and smooth compression



El Rafei et al. 2019



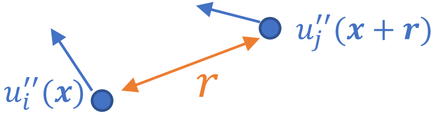


Summary

- BHR-4
  - Improvements seen over BHR3.1 in problems with stabilized mixing layers
    - BHR-4.0 also captures the behavior of certain variables such as $\bar{u}_i = \tilde{u}_i - a_i$ that BHR-3.1 doesn't reliably capture
  - Good agreement with DNS/LES in a range of classical problems
  - Minimal added model complexity relative to BHR3.1
- Possible Issues
  - Realizability
    - Hard to enforce a_i^k and $b^k \rightarrow 0$ as $\tilde{c}^k \rightarrow 0$
  - Cost
    - Depends on the problem, but usually not significantly different

Local Wavenumber Model (LWN)

- Tracks two-point correlations
  - BHR Reynolds stress, representing turbulent kinetic energy
    - $\tilde{R}_{ij}(\boldsymbol{x}) = \dfrac{\overline{\rho(\boldsymbol{x}) u_i''(\boldsymbol{x})\, u_j''(\boldsymbol{x})}}{\overline{\rho}(\boldsymbol{x})}$
  - LWN Reynolds stress, represent velocity correlations at some separation scale
    - $\tilde{R}_{ij}(\boldsymbol{x}, \boldsymbol{r}) = \dfrac{\overline{\rho(\boldsymbol{x}) u_i''(\boldsymbol{x})\, u_j''(\boldsymbol{x}+\boldsymbol{r})}}{\overline{\rho}(\boldsymbol{x})}$



- In practice, evolves spectral quantities at every grid cell $\tilde{R}_{ij}(\boldsymbol{x}, k)$, $a_i(\boldsymbol{x}, k)$, $b(\boldsymbol{x}, k)$
  - Inherently includes lengthscale information, no need for explicitly evolved lengthscales
  - Simpler initial conditions and transition to turbulence
  - Increased model complexity.
    - $LWN(x,k,t) = \underbrace{physical\_space\_evolution(x,k,t)}_{\text{BHR-like, TKE production by pressure gradients, etc., ..}} + \underbrace{spectral\_evolution(x,k,t)}_{\text{Evolution of scales, } k^{-\frac{5}{3}} \text{ cascade, …}}$

Multispecies Material Transport (BHR4.0)

- Still track slightly modified BHR3.1 a and b equations
  - $\frac{\partial(\bar{\rho}a_i)}{\partial t} + (\bar{\rho}\tilde{u}_k a_i)_{,k} = b\,\bar{P}_{,j} - \tilde{R}_{ik}\bar{\rho}_{,k} - \rho a_k \bar{u}_{i,k} + \bar{\rho}\frac{C_\mu}{\sigma_a}\left(S_T\sqrt{K}a_{i,k}\right)_{,k} - C_{ap}b\bar{P}_{,i} + C_{au}\bar{\rho}a_k\bar{u}_{i,k} - \bar{\rho}\frac{\sqrt{K}}{S_D}C_{a1}a_i$
  - $\frac{\partial(\bar{\rho}b)}{\partial t} + (\bar{\rho}b\tilde{u}_k)_{,k} = -2(b+1)a_k\bar{\rho}_{,k} + 2\bar{\rho}a_n b_{,n} + \bar{\rho}^2\frac{C_\mu}{\sigma_b}\left(\frac{1}{\bar{\rho}}S_T\sqrt{K}b_{,n}\right)_{,n} - C_{b1}\bar{\rho}\frac{\sqrt{K}}{S_D}(1+b)b$

$a_i = \sum_k \frac{a_i^k}{\rho^k}$ if $\nabla \cdot \bar{u}=0$

- Multispecies a^k and b^k equations
  - $\frac{\partial\bar{\rho}a_i^k}{\partial t} + \left(\bar{\rho}\tilde{u}_j a_i^k\right)_{,j} = (C_{au}-1)\bar{\rho}a_j^k\bar{u}_{i,j} + \bar{\rho}\tilde{R}_{ij}\tilde{c}_{,j}^k - b^k(1-C_{ap})\bar{P}_{,i} + C_\mu\left(S_T\sqrt{K}(\bar{\rho}a_i^k)_{,j}\right)_{,j} + a_j\left(\bar{\rho}a_i^k\right)_{,j} - C_{a1}\bar{\rho}\frac{\sqrt{K}}{S_D}a_i^k$
  - $\frac{\partial\bar{\rho}b^k}{\partial t} + \left(\bar{\rho}\tilde{u}_j b^k\right)_{,j} = \bar{\rho}a_j\left(c^k + 2b^k\right)_{,j} + \bar{\rho}b^k a_{j,j} - a_j^k\bar{\rho}_{,j} - \bar{\rho}C_\mu\left(\frac{1}{\bar{\rho}}S_T\sqrt{K}\left(\bar{\rho}b^k\right)_{,j}\right)_{,j} - C_{b1}\bar{\rho}\frac{\sqrt{K}}{S_D}(1+b)b^k$